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The Schrödinger–Poisson Eigenmatrix Problem

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1. INTRODUCTION

In the present paper we study solutions to the periodic Schrödinger–Poisson (SP) System as treated in [1], except that we consider stationary states, i.e., solutions of the form ($\hbar = 1$)

$$\Psi(x, t) = e^{-iEt}\Phi(x). \tag{1.1}$$

Here Ψ and Φ are vector functions [1] and E is a matrix.

The Schrödinger–Poisson system satisfied by Φ will be time-independent if certain conditions are satisfied by E; this matrix is a generalization of the usual energy eigenvalue of elementary quantum mechanics.

This problem with constant E was studied in [2, 3]. The case in which E is a diagonal matrix has been considered in papers by Nier [4] and by Albinus *et al.* [5]. Nier has proved existence of unique solutions of the SP system for both periodic and Dirichlet data. His technique involves studying a variational problem for the potential V; a similar technique is used in [5], where only Dirichlet data are considered. Our technique involves the solution of the nonlinear eigenvalue problem for the Schrödinger equation using a fixed point argument; we restrict our attention to periodic boundary conditions.

We remark that we attach physical significance to the off-diagonal matrix elements of E—as transition probabilities which obey a condition

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of detailed balance [6, p. 33]. The eigenvalues of E, denoted by μ_m, are taken to be the energies of the various eigenstates.

In this paper we prove that there exists at least one space-periodic solution (Φ, V) of the Schrödinger–Poisson eigenmatrix problem. In Section 2, the problem is formulated, necessary conditions for the eigenmatrix are derived, and a diagonalization procedure is presented. In Section 3 we prove the existence theorem using a Schauder fixed-point argument, and derive bounds for the eigenvalues μ_m of E. We also present an iteration scheme of linear equations for the approximations of the eigenvalues; using minimax principles, it is not necessary to solve for the eigenstates.

As one easily shows, the eigenmatrix does not appear in the stationary Wigner equation, so in this case the usual isomorphism between Schrödinger and Wigner equation [7] no longer holds. In fact, the stationary Wigner equation apparently does not have a unique solution, for example, in that any function of the Hamiltonian can generate a solution [8]. (These solutions are the analogue of the BGK modes formula in classical Vlasov theory [9].) For this reason, we restrict our attention to SP.

According to a result of Nier [4], the potential V of SP is unique in the space $H^1_{per}(Q)/\mathbb{R}$, where $Q = Q_L$ is the cube $[0, L]^d \subset \mathbb{R}^d$, $d = 1, 2, 3$.

2. FORMULATION OF THE PROBLEM

The SP system describes the time evolution of the vector $\Psi = (\psi_m)_{m \in \mathbb{N}}$. It can be written (see, for example, [10, 11])

$$i\Psi_t = -\frac{1}{2}\Delta\Psi + V(\Psi)\Psi + \tilde{V}\psi \tag{2.1a}$$

$$-\Delta V(\Psi) = n_\Psi - n_D \tag{2.1b}$$

$$n_\Psi(x, t) = \sum \lambda_m |\psi_m|^2 \tag{2.1c}$$

$$0 \le \lambda_m \le 1, \qquad \sum \lambda_m = 1. \tag{2.1d}$$

We shall denote by Λ the sequence $(\lambda_m)_{m \in \mathbb{N}}$. The system (2.1) is to be solved subject to periodic boundary conditions on the cube Q_L; λ_m is the probability of the state ψ_m. $\tilde{V}$ is a given external potential depending only on x, while n_D is a given background charge density, also depending only on x. Assumptions on $\tilde{V}$ and n_D are given in Section 3. This system, or similar systems, has been used to model various semiconductor devices for which quantum effects are important [12–14].

We study SP in the Hilbert spaces Y^k (see Section 3) and

$$X_\Lambda^k = \left\{\Psi = (\psi_m)_{m\in\mathbb{N}} | \psi_m \in H_{loc}^k(\mathbb{R}^d); \forall x \in Q_L, \forall m \in \mathbb{N}, \forall l \in \mathbb{Z}^d, \psi_m(x+lL) = \psi_m(x)\right\} \quad (2.2)$$

(The periodicity condition is understood in the L^2 sense.) The inner product in X_Λ^k is

$$(\Psi, \Phi)_{k,\Lambda} = \sum_{m=1}^{\infty} \lambda_m \sum_{|\alpha|\le k} (\partial^\alpha \psi_m, \partial^\alpha \phi_m)_{L^2(Q_L)}. \quad (2.3)$$

When we substitute (1.1) into (2.1), write $\Phi = (\phi_m)_{m\in\mathbb{N}}$, we should like to recover a stationary equation. Noting Eqs. (2.1b) and (2.1c), this requires that E be self-adjoint in the Hilbert space

$$l_\Lambda^2 = \left\{\xi = (\xi_m)_{m\in\mathbb{N}} \Big| \sum_{n=1}^{\infty} \lambda_n |\xi_n|^2 < \infty\right\} \quad (2.4a)$$

with inner product

$$(\zeta, \eta)_\Lambda = \sum_{m=1}^{\infty} \lambda_m \zeta_m \overline{\eta}_m. \quad (2.4b)$$

Then e^{iEt} will be unitary in l_Λ^2 and [cf. (2.1c)] $n_\Psi = n_\Phi$, implying $V(\Psi) = V(\Phi)$.

A simple calculation shows that E will be self-adjoint in l_n^2 if and only if

$$\lambda_n \overline{E}_{nk} = \lambda_k E_{kn}. \quad (2.5)$$

If we interpret E_{nk} as a transition matrix element from the state ϕ_n to the state ϕ_k, then (2.5) is the condition of microscopic irreversibility or "detailed balance" [6, 15].

The following system, then, is obtained for Φ,

$$-\frac{1}{2}\Delta\Phi + V(\Phi)\Phi + V\Phi = E\Phi \quad (2.6a)$$

$$-\Delta V(\Phi) = n_\Phi - n_D, \quad (2.6b)$$

where the unitarity of e^{iEt} on l_Λ^2 has been used. In addition to the detailed balance condition on E, we need to assume that E has a pure point spectrum in l_Λ^2 in order to prove existence of solutions.

With these assumptions, E can be diagonalized by a unitary transformation U on l^2_Λ such that

$$U^{-1}EU = M = \operatorname{diag}(\mu_m)_{m\in\mathbb{N}} \tag{2.7a}$$

and

$$\tilde{\Phi} = U^{-1}\Phi \tag{2.7b}$$

(so that the solution we seek is $U\tilde{\Phi}$). We arrive at the same set of equations (2.6) for $\tilde{\Phi}$, but with E replaced by M (noting that V is invariant under U). For convenience we write Φ instead of $\tilde{\Phi}$. Then the equations we wish to solve are

$$-\frac{1}{2}\Delta\phi_m + V(\Phi)\phi_m + \tilde{V}\phi_m = \mu_m\phi_m \tag{2.8a}$$

$$-\Delta V(\Phi) = n_\Phi - n_D \tag{2.8b}$$

$$n_\Phi = \sum \lambda_m(\mu_m)|\phi_m|^2. \tag{2.8c}$$

For the time-dependent problem, the set $\Lambda = (\lambda_m)_{m\in\mathbb{N}}$ is datum [10, 11]. For the eigenproblem, on the other hand, the λ_m are functions of the energy eigenvalues μ_m, for example, the Fermi distribution [4, 5, 12, 13]. We always have to enforce the normalization $\sum_{m\in\mathbb{N}}\lambda_m(\mu_m) = 1$. Other distributions beside the Fermi one could be used (for example, the Boltzmann distribution $\sim e^{-\mu_m}$). It is merely required that the $\lambda_m(M)$ be strictly monotonically decreasing sufficiently rapidly (plus some other regularity assumptions).

3. THE FIXED-POINT ARGUMENT

We begin by defining sequence spaces $l(F)$ as the set of all sequences $\phi = (\varphi_m)_{m\in\mathbb{N}}$, $\varphi_m \in F$, and F is a Banach space. With the metric

$$d(\phi,\psi) = \sum_{j=1}^{\infty} 2^{-j}\frac{\|\varphi_j - \psi_j\|_F}{1 + \|\varphi_j - \psi_j\|_F}$$

$l(F)$ is a Fréchet space (i.e., a complete locally convex metric space; cf. [16, p. 287; 17, p. 54]; for a Cartesian product of sequence spaces, we impose the Cartesian product metric).

Let

$$Y^k = l\left(H^k_{per}(Q_L)\right) \times l(\mathbb{R}), \qquad k \in \mathbb{N}_0 = N \cup \{0\}.$$

To define the operator T whose fixed point we seek in Y^1, some technical assumptions are necessary on the functions $\lambda_m(t)$ for dimensions $d = 1, 2, 3$: Let

$$\lambda_m(t) = \frac{\tilde{\lambda}_m(t)}{\Lambda(t)}, \tag{3.1a}$$

where

$$\Lambda(\mu) \coloneqq \sum_{m \in \mathbb{N}} \tilde{\lambda}_m(\mu_m), \tag{3.1b}$$

with $t \in \mathbb{R}$, $\mu = (\mu_m)_{m \in \mathbb{N}}$. Then we assume

(Λ_1) For each $m \in \mathbb{N}$, $\tilde{\lambda}_m(t)$ is a continuous, positive, decreasing function of t;

(Λ_2) $0 < c^* \coloneqq \sum_{m \in \mathbb{N}} \tilde{\lambda}_m((c^{(1)}/2L^2)m^{2/d})m^{1/2} < \infty$, where $c^{(1)} > 0$ is a universal constant to be specified later (Lemma 3.2); let us define $\mu^{(j)}(\gamma)$, $j = 1, 2$, by $\mu_m^{(1)}(\gamma) = (c^{(1)}/L^2)m^{2/d} - \gamma$, $\mu_m^{(2)}(\gamma) = (c^{(2)}/L^2)m^{2/d} + \gamma$, where $c^{(2)} > 0$ is another universal constant also introduced in Lemma 3.2;

(Λ_3) $n_D \in L^2_{per}(Q_L), \tilde{V}$ real, and $\tilde{V} \in L^\infty_{per}(Q_2)$.

Let us note some consequences of (Λ_1) and (Λ_2). First, we have

$$0 < \tilde{c} \coloneqq \Lambda(\tilde{\mu}) \leq c^* < \infty \tag{3.2a}$$

for $\tilde{\mu} = (\tilde{\mu}_m)$, $\tilde{\mu}_m \coloneqq (c^{(1)}/2L^2)m^{2/d}$. Also, for all $\gamma > 0$

$$0 < \Lambda\big(\mu^{(1)}(\gamma)\big) < \infty \tag{3.2b}$$

since, with $N(\gamma) \coloneqq [(2L^2/c^{(1)})\gamma]^{d/2}$

$$\sum_{m \geq N(\gamma)} \tilde{\lambda}_m\big(\mu_m^{(1)}(\gamma)\big) \leq \sum_{m \geq N(\gamma)} \tilde{\lambda}_m\left(\frac{c^{(1)}}{2L^2}m^{2/d}\right) \leq \tilde{c},$$

so that

$$0 < \Lambda(\mu) < \infty \tag{3.2c}$$

for any sequence $\mu = (\mu_m)$ s.t. $\mu_m \geq \mu_m^{(1)}(\gamma)$. (Furthermore, let us mention that (Λ_1) could be weakened to include cases where the $\tilde{\lambda}_m(t)$ are non-negative, but we do not consider this here.)

The most important special case where $(\Lambda_1), (\Lambda_2)$ are satisfied is that of the Fermi function

$$\tilde{\lambda}_m(t) = \frac{c_m}{e^{\alpha(t-\mu_F)} + 1}$$

with a bounded, strictly positive sequence (c_m) which contains physical parameters such as mass, temperature, Boltzmann and Planck constants, etc., α is the inverse temperature and μ_F is the so-called Fermi level.

LEMMA 3.1. *Let* $(\Phi, \mu) \in Y^1$ *and* $\|\Phi\|_{L^4}^2 := \sum_{m\in\mathbb{N}} \lambda_m(\mu_m)\|\phi_m\|_{L^4(Q)}^2 < \infty$. *Then the Poisson equation* (2.8b) *has a solution* $V \in H_{per}^2(Q_L)/\mathbb{R}$ *s.t.*

$$\|V\|_{L^\infty} \le V_0 + CL^2\left\{\|n_0\|_{L^2} + \|\Phi\|_{L^4}^2\right\} \tag{3.3}$$

with a generic constant $C > 0$ *and an arbitrary constant* $V_0 \ge 0$.

Proof. Let $\tilde{n} = n_\Phi - n_D$ [cf. (2.1b)]. Then introducing the Fourier basis $\{h_k\}_{k\in\mathbb{Z}^d}$ with $h_k(x) = L^{-d/2}\exp((2\pi i/L)k\cdot x)$, the Fourier coefficients of $\tilde{n} = n_\Phi - n_D$ are

$$\tilde{n}_k = (\tilde{n}, h_k) = \int_0^L \tilde{n}_k(x)\bar{h}_k(x)\,dx.$$

Then

$$V = V_0 + \frac{L^2}{4\pi^2}\sum_{k\in\mathbb{Z}^d/\{0\}} \frac{\tilde{n}_k}{k^2}h_k \qquad (V_0 \in \mathbb{R})$$

is a solution of (2.8b) in $H_{per}^2(Q_L)$. (Note that the charge neutrality condition implies $\tilde{n}_0 = 0$). The L^∞ estimates follows from

$$\|V\|_{L^\infty} \le \|V_0\|_{L^\infty} + \frac{L^2}{4\pi^2}\left\{\sum_{k\in\mathbb{Z}^d\setminus\{0\}}\frac{1}{k^4}\right\}^{1/2}\left\{\sum_{k\in\mathbb{Z}^d}|\tilde{n}_k|^2\right\}^{1/2}$$

and

$$\begin{aligned}\left\{\sum_{k\in\mathbb{Z}^d}|\tilde{n}_k|^2\right\}^{1/2} &= \|\tilde{n}\|_{L^2} \le \|n_D\|_{L^2} + \|n_\Phi\|_{L^2}\\ &\le \|n_D\|_{L^2} + \sum\lambda_m(\mu_m)\|\phi_m\|_{L^4}^2.\end{aligned}$$

LEMMA 3.2. *Let* $V \in L_{per}^\infty(Q_L)$ *and real. Then the linear eigenvalue system*

$$-\tfrac{1}{2}\Delta\varphi_m + V\varphi_m = \mu_m\varphi_m, \qquad m\in\mathbb{N} \tag{3.4}$$

has a solution sequence $(\Phi, \mu) \in Y^2$ *where* $\Phi = (\varphi_m)_{m \in \mathbb{N}}$ *is an orthonormal system in* $L^2_{per}(Q)$; *the eigenvalues* $\mu = (\mu_m)_{m \in \mathbb{N}}$ *are real, arranged in increasing order and fulfill* $\mu_m \to \infty$ *for* $m \to \infty$. *Furthermore, there are positive generic constants* $c^{(1)}, c^{(2)} > 0$ *such that the estimate*

$$-\|V\|_\infty + \frac{c^{(1)}}{L^2} m^{2/d} \le \mu_m \le \frac{c^{(2)}}{L^2} m^{2/d} + \|V\|_\infty \tag{3.5}$$

is valid.

Proof. The existence follows from well-known results of the theory of elliptic differential equations [19] and the minimax characterization of eigenvalues of self-adjoint linear operators, see [19, pp. 446 ff] or [20]. In the proof of (3.5), we first consider the case $V = 0$ and $L = 2\pi$. Then the proof of the lower bound in (3.5) can be found in [19, Appendix, Proposition 4.1]. Using similar notation and counting the eigenvalues according to multiplicity we have (still for $V = 0$)

$$0 \le \mu_1 \le \mu_2 \le \cdots \le \mu_m \le, \ldots, \qquad \mu_m \to \infty \quad \text{for} \quad m \to \infty. \tag{3.6}$$

We define for $p \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$

$$\mathscr{E}_p = \left\{ l \in \mathbb{N}_0^d \middle| \sum_{\substack{\alpha \in \mathbb{N}_0^d \\ |\alpha| = 1}} l_1^{2\alpha_1} + \cdots + l_d^{2\alpha_d} \le p \right\} \tag{3.7}$$

(for $d = 1, 2, 3$); let N_p be the cardinality of $\mathscr{E}_p$. By definition the $\mathscr{E}_p$ consist of $\mu_1, \ldots, \mu_{N_p}$, thus $\mu_{N_p} \le N_p$. We now prove the inequality

$$N_p \ge c^* p^{d/2} \tag{3.8}$$

with a finite constant $c^* > 0$ (depending only on d). Let Q^* be the largest cube with center at zero inscribed in the ball with center at zero and radius $\sqrt{p}$. The side L^* of this cube is proportional to $\sqrt{p}$. This implies that there are at least $([L^*] + 1)$ eigenvalues in the ball. This proves (3.8).

Now let m be given and let q be the smallest integer $\ge (m/c^*)^{2/d}$; further, set $q_1 = [c^* q^{d/2}]$. Then $m \le q_1$ and by monotonicity we arrive at

$$\mu_m \le \mu_{q_1} \le \mu_{N_q} \le q < \left(\frac{m}{c^*}\right)^{2/d} + 1 \le c m^{2/d}.$$

Here we have used $q_1 \le N_q$ together with (3.7) for the case $V = 0$.

Applying both the minimax method and the comparison principle for eigenvalues [19, 20], we see that (3.5) follows for any bounded potential V, the constants depending only on d (for the case $L = 2\pi$). For arbitrary L, (3.5) is obtained by a simple scaling argument.

Remark. We may write (3.5) also in the form

$$-\|V\|_\infty + c^{(1)}\left(\frac{m}{|Q_L|}\right)^{2/d} \le \mu_m \le \|V\|_\infty + c^{(2)}\left(\frac{m}{|Q_L|}\right)^{2/d}.$$

We now introduce the fixed point operator T and the set $S \subset Y^1$ s.t. $T\colon S \to S$ has a fixed point in S. Let $\gamma \ge \gamma_0$ be a positive constant to be specified later and $c^{(1)}, c^{(2)}$ be the constants from Lemma 3.2; $\mu^{(1)}(\gamma) = (\mu_m^{(1)}(\gamma))$ as defined in (Λ_2). Then set

$$S = S_\gamma = \Big\{(\Phi, \mu) \in Y^1 | \Phi = (\varphi_m)_{m\in\mathbb{N}},\ \mu = (\mu_m)_{m\in\mathbb{N}},\ \|\varphi_m\|_{L^2} \le 1;$$
$$\|\nabla\varphi_m\|_{L^2} \le K_m(\gamma) = \left(\gamma + \frac{2c^{(2)}}{L^2} m^{2/d}\right)^{1/2},\ \mu_m^{(1)}(\gamma) \le \mu_m,\ \forall m \in \mathbb{N}\Big\}. \tag{3.9}$$

Evidently S is a convex subset of Y^1. For $(\Phi, \mu) \in S$, let

$$T(\Phi, \mu) = (\tilde{\Phi}, \tilde{\mu}),$$

where $\tilde{\Phi} = (\pm\tilde{\varphi}_m)_{m\in\mathbb{N}}$, $\tilde{\mu} = (\tilde{\mu}_m)_{m\in\mathbb{N}}$ with $\tilde{\varphi}_m$ and $-\tilde{\varphi}_m$ associated with the same $\tilde{\mu}_m$ ($\forall_m \in \mathbb{N}$); the (φ_m, μ_m) are the orthonormal solutions of the linear eigenvalue problem

$$-\tfrac{1}{2}\Delta\tilde{\varphi}_m + \big(V(\Phi) + \tilde{V}\big)\tilde{\varphi}_m = \tilde{\mu}_m\tilde{\varphi}_m. \tag{3.10}$$

($\forall m \in \mathbb{N}$) with L-periodic boundary conditions on Q where $V(\Phi)$ is given by Poisson's equation (2.8b). Later, in proving continuity of T, we are confronted with the fact that both $\pm\tilde{\varphi}_m$ are normalized eigenfunctions with the same eigenvalue $\tilde{\mu}_m$, a fact which must be incorporated into the definition of T, but in proving the other properties of Lemma 3.3 we will ignore it (since S_γ is invariant under the transformation $\varphi_m \to -\varphi_m$). From Lemmata 3.1 and 3.2 it follows that T is well-defined on S.

LEMMA 3.3. *Let conditions* (Λ_1)–(Λ_3) *hold. Then there is a constant* $\gamma > 0$ *s.t.* $T(S_\gamma) \subset S_\gamma$. *Further, T is continuous on S_γ and $T(S_\gamma)$ is relatively compact on Y^1.*

For the proof of the crucial Lemma 3.3 we need the technical

LEMMA 3.4. *There exists a generic constant $C > 0$ (not depending on L) such that for any $\varphi \in H^1_{per}(Q_L)$*

$$\|\varphi\|_{L^4(Q_L)} \le C\Big\{L^{d/4}\|\varphi\|_{L^2(Q_L)} + \|\nabla\varphi\|^{d/4}_{L^2(Q_L)}\|\varphi\|^{1-d/4}_{L^2(Q_L)}\Big\}. \tag{3.11}$$

Proof. The result follows from the Gagliardo–Nirenberg inequality [1, 18] for functions with mean value zero. The independence of C on L follows from a scaling argument.

Proof of Lemma 3.3. Let $(\Phi, \mu) \in S_\gamma$ with $\gamma > \gamma_0$ [cf. (Λ_1)–(Λ_3)]. Choosing $V_0 = 0$ in Lemma 3.1, using the definition of S_γ and Eq. (3.2) we get that $\sum_{m \in \mathbb{N}} \tilde{\gamma}_m(\mu_m)$ converges (since $\mu_m \geq \mu_m^{(1)}(\gamma)$). Thus $\sum_{m \in \mathbb{N}} \lambda_m(\mu_m) = 1$ and furthermore

$$4\|V(\Phi)\|_{L^\infty} \leq 4CL^2 \left\{ \|n_D\|_{L^2} + C^2 \sum_{m \in \mathbb{N}} \lambda_m(\mu_m) \left[L^{d/4} + K_m^{d/4} \right]^2 \right\}$$

$$\leq 4CL^2 \|n_D\|_{L^2} + 8C^3 L^2 \sum_{m \in \mathbb{N}} \lambda_m(\mu_m) \left(\gamma + \frac{2c^{(2)}}{L^2} m^{2/d} \right)^{d/4}. \tag{3.12}$$

If we denote the last term in (3.12) by J we have $J = J_1 + J_2$, where J_1 is the sum over all $m \leq N(\gamma)$ and J_2 the remainder. [See (3.2b) for the definition of $N(\gamma)$.]

Now we arrive at

$$J_1 \leq \sum_{m \leq N(\gamma)} \lambda_m(\mu_m) \left[1 + \frac{4c^{(2)}}{c^{(1)}} \right]^{d/4} \gamma^{d/4} \leq \tilde{c}_1 \gamma^{d/4} \tag{3.13}$$

(with $\tilde{c}_1 := (1 + 4c^{(2)}/c^{(1)})^{d/4}$),

$$J_2 \leq \sum_{m \geq N(\gamma)} \lambda_m(\mu_m) \left[\frac{c^{(1)}}{L^2} + \frac{2c^{(2)}}{L^2} \right]^{d/4} m^{1/2}$$

$$\leq \frac{\tilde{c}_2 \sum_{m \geq N(\gamma)} \tilde{\lambda}_m\big((c^{(1)}/2L^2) m^{2/d}\big) m^{1/2}}{\sum_{m \leq N(\gamma)} \tilde{\lambda}_m\big((c^{(1)}/2L^2) m^{2/d}\big)} \tag{3.14}$$

(where $\tilde{c}_2 := [c^{(1)} + 2c^{(2)}]^{d/4} L^{-d/2}$).

By (3.2a) we can choose an appropriate $\gamma_0 > 0$ s.t. for $\gamma \geq \gamma_0$ the sum in the denominator of (3.14) is $\geq \tilde{c}/2$; then using (Λ_2) we get

$$J_2 \leq 2\tilde{c}_2 \frac{c^*}{\tilde{c}}$$

which finally implies that for all $\gamma \geq \gamma_1 \geq \gamma_0$ (with an appropriate γ_1)

$$4\|V(\Phi)\|_{L^\infty} + 4\|\tilde{V}\|_{L^\infty} \leq 4\|\tilde{V}\|_{L^\infty} + 4CL^2\|n_D\|_{L^2} + 8C^3L^{d/2+2} + C^3L^2\tilde{c}_2\frac{c^*}{\tilde{c}} + 8C^3L^2\tilde{c}_1\gamma^{d/4} \leq \gamma. \tag{3.15}$$

From Lemma 3.2, we get, for all $m \in \mathbb{N}$

$$\frac{1}{2}\int_Q |\nabla\varphi_m|^2\,dx = -\int_Q \big(V(\Phi) + \tilde{V}\big)|\varphi_m|^2\,dx + \tilde{\mu}_m. \tag{3.16}$$

Since by Lemma 3.2 we have also

$$\tilde{\mu}_m \leq \frac{c^{(2)}}{L^2}m^{2/d} + \|\tilde{V}\|_{L^\infty} + \|V(\Phi)\|_{L^\infty}$$

we obtain from (3.16) and (3.15) for all $m \in \mathbb{N}$

$$\begin{aligned}\|\nabla\tilde{\varphi}_m\|_{L^2}^2 &\leq 4\|V(\Phi)\|_{L^\infty} + 4\|\tilde{V}\|_{L^\infty} + \frac{2c^{(2)}}{L^2}m^{2/d}\\ &\leq \gamma + \frac{2c^{(2)}}{L^2}m^{2/d} \leq K_m^2.\end{aligned}$$

Thus, we have again by Lemma 3.2 and Eq. (3.15) that $\|\tilde{\varphi}_m\|_{L^2} = 1$ and

$$\begin{aligned}\tilde{\mu}_m &\geq \frac{c^{(1)}}{L^2}m^{2/d} - \|V(\Phi) + \tilde{V}\|_{L^\infty}\\ &\geq \frac{c^{(1)}}{L^2}m^{2/d} - \big(\|V(\Phi)\|_{L^\infty} + \|\tilde{V}\|_{L^\infty}\big) \geq \frac{c^{(1)}}{L^2}m^{2/d} - \gamma = \mu_m^{(1)}(\gamma);\end{aligned}$$

similarly, $\tilde{\mu}_m \leq \mu_m^{(2)}(\gamma)$. Thus $T(S_\gamma) \subset S_\gamma$.

We now show that $T(S_\gamma)$ is relatively compact in Y^1. Since Y^1 is a metric space, it is sufficient to show sequential compactness of $T(\Phi^{(N)}, \mu^{(N)}) = (\tilde{\Phi}^{(N)}, \tilde{\mu}^{(N)})$ for a sequence $(\Phi^{(N)}, \mu^{(N)})_{N\in\mathbb{N}} \subset S_\gamma$. Let $\Phi^{(N)} = (\varphi_m^{(N)})$, $\mu^{(N)} = (\mu_m^{(N)})$, and similarly for $\tilde{\Phi}^{(N)}$ and $\tilde{\mu}^{(N)}$. We show that the H^2-norm of each component sequence $(\tilde{\varphi}_m^{(N)})$, m fixed, is bounded. This follows from Lemma 3.2 and the definition of S_γ since

$$\|\tilde{\varphi}_m^{(N)}\|_{L^2} = 1, \qquad \|\nabla\tilde{\varphi}_m^{(N)}\|_{L^2} \leq K_m(\gamma).$$

From

$$-\tfrac{1}{2}\Delta\tilde{\varphi}_m^{(N)} + \big(V(\Phi^{(N)}) + \tilde{V}\big)\tilde{\varphi}_m^{(N)} = \tilde{\mu}_m^{(N)}\tilde{\varphi}_m^{(N)}$$

we obtain

$$\begin{aligned}\left\|\Delta\tilde{\varphi}_m^{(N)}\right\|_{L^2} &\le 2\left(\left\|V(\Phi^{(N)})\right\|_{L^\infty}+\|\tilde{V}\|_{L^\infty}\right)+2\tilde{\mu}_n^{(N)}\\ &\le \frac{\gamma}{2}+\frac{2c^{(2)}}{L^2}m^{2/d}+2\gamma=2K_m^2(\gamma)+\frac{\gamma}{2}.\end{aligned}\tag{3.17}$$

Since H^2_{per} is compactly embedded in H^1_{per}, each component-sequence $(\tilde{\varphi}_m^{(N)})$ has a subsequence which converges in $H^1_{per}(Q_L)$; the same is true of the component-sequence $(\tilde{\mu}_m^{(N)})_{N\in\mathbb{N}}$, since by Lemma 3.2 we have an estimate of the type $|\tilde{\mu}_m^{(N)}|\le\alpha_m$ $(\forall m\in\mathbb{N})$. By the definition of the topology of Y^1, a diagonalization procedure gives a subsequence of $(\tilde{\Phi}^{(N)},\tilde{\mu}^{(N)})$ which converges in the topology of Y^1.

To prove continuity of T on S_γ, again it is enough to deal with sequences. Thus, let $(\Phi^{(N)},\mu^{(N)})\to(\Phi,\mu)\in S_\gamma$ on Y^1. We first show that

$$V(\Phi^{(N)})\to V(\Phi)\tag{3.18}$$

in $L^\infty(Q)$; we have

$$-\Delta\left(V(\Phi^{(N)})-V(\Phi)\right)=n_{\Phi^{(N)}}-n_\Phi$$

and by Lemma 3.1

$$\begin{aligned}\left\|V(\Phi^{(N)})-V(\Phi)\right\|_{L^\infty} &\le C_L\sum_{m\in\mathbb{N}}\lambda_m(\mu_m^{(N)})\left\||\varphi_m^{(N)}|^2-|\varphi_m|^2\right\|_{L^2}\\ &\quad+C_L\sum_{m\in\mathbb{N}}\left|\lambda_m(\mu_m^{(N)})-\lambda_m(\mu_m)\right|\|\varphi_m\|^2_{L^4}\\ &=: R_1^{(N)}+R_2^{(N)}.\end{aligned}$$

We first see that

$$\Lambda(\mu^{(N)})\to\Lambda(\mu),\qquad N\to\infty\tag{3.19}$$

because for any $\epsilon>0$ there is an integer N_1 (which depends on ϵ) s.t. [cf. Eq. (3.2)]

$$2\sum_{m\ge N_1+1}\tilde{\lambda}_m(\mu_m^{(1)}(\gamma))<\epsilon/2;$$

now choose N_2 (depending on ϵ) s.t. for $m=1,\dots,N_1$

$$\left|\tilde{\lambda}_m(\mu_m^{(N)})-\tilde{\lambda}_m(\mu_m)\right|<\frac{\epsilon}{2N_1}\qquad\text{for all } N\ge N_2;$$

this gives

$$\left|\Lambda(\mu^{(N)}) - \Lambda(\mu)\right| \le \sum_{m \le N_1(\epsilon)} \left|\tilde{\lambda}_m(\mu_m^{(N)}) - \tilde{\lambda}_m(\mu_m)\right|$$

$$+ 2 \sum_{m \ge N_1(\epsilon)+1} \tilde{\lambda}_m\left(\mu_m^{(1)}(\gamma)\right) < \epsilon,$$

for $N \ge N_2$. This implies (3.19).

Using the definition of S_γ and Lemma 3.4 we get analogously (with same notation for N_1 and N_2 as above)

$$R_1^{(N)} \le 2 \sum_{m \le N_1} \|\varphi_m^{(N)} - \varphi_m\|_{L^2}$$

$$+C(\gamma) \frac{\sum_{m \ge N_1+1} \tilde{\lambda}_m\left(\mu_m^{(1)}(\gamma)\right)}{\tilde{\lambda}_1\left(\mu_1^{(2)}(\gamma)\right)} < \epsilon$$

for $N \ge N_2$. Also

$$R_2^{(N)} \le C(\gamma) \sum_{m \in \mathbb{N}} \frac{\left|\tilde{\lambda}_m(\mu_m^{(N)}) - \tilde{\lambda}_m(\mu_m)\right|}{\left|\Lambda(\mu^{(N)})\right|}$$

$$+ C(\gamma) \frac{\left|\Lambda(\mu^{(N)}) - \Lambda(\mu)\right|}{\Lambda(\mu^{(N)}) \cdot \Lambda(\mu)} \sum_{m \in \mathbb{N}} \tilde{\lambda}_m(\mu_m)$$

$$\le \frac{C(\gamma)}{\tilde{\lambda}_1\left(\mu_1^{(2)}(\gamma)\right)} \left\{ \sum_{m \le N_1} + \sum_{m \ge N_1+1} \right\} \left|\tilde{\lambda}_m(\mu_m^{(N)}) - \tilde{\lambda}_m(\mu_m)\right|$$

$$+ \tilde{c}(\gamma) \left|\Lambda(\mu^{(N)}) - \Lambda(\mu)\right| < \epsilon$$

for $N \ge N_2$. This implies (3.18).

Let us now assume that there is a subsequence of $(\tilde{\Phi}^{(N)}, \tilde{\mu}^{(N)})_{N \in \mathbb{N}}$ which does not converge to $(\tilde{\Phi}, \tilde{\mu})$ in Y^1. (We denote the subsequence with the same notation as the sequence.)

By the compactness of $T(S_\gamma)$ we may assume that $(\tilde{\Phi}^{(N)}, \tilde{\mu}^{(N)}) \to (\Psi, \nu) \in S_\gamma$ in Y^1 for $N \to \infty$. Since $V(\Phi^{(N)}) \to V(\Phi)$ in $L^\infty(Q_L)$ for $N \to \infty$, the (ψ_m, ν_m) are weak solutions of the normalized eigenvalue problem for the Schrödinger operator $-\frac{1}{2}\Delta + (V(\Phi) + \tilde{V})$ (with L-periodic boundary conditions on Q, and then by elliptic regularity theory are also strong solutions in $H^2_{per}(Q_L)$ (cf. [18]). This implies that up to a possible reordering, the $(\pm\psi_m, \nu_m)$ are equal to the $(\pm\tilde{\varphi}_m, \tilde{\mu}_m)$, that is, $(\tilde{\Phi}^{(N)}, \tilde{\mu}^{(N)}) \to (\tilde{\Phi}, \tilde{\mu})$ which is a contradiction. This concludes the proof of the lemma.

Using the Schauder–Tychonov fixed-point theorem for locally convex topological vector spaces [21, p. 230], we conclude from Lemma 3.3

THEOREM 3.5. *Let* (Λ_1)–(Λ_3) *hold, and let* $d = 1, 2, 3$. *Then the Schrödinger–Poisson eigenvalue problem* (2.8) *has a solution* (Φ, μ) *in* Y^2.

From the theorem, the definition of S_γ, and (3.17) follows

COROLLARY 3.6. *Let the assumptions of Theorem* 3.5 *be true, and assume furthermore that*

$$\sum_{m \in \mathbb{N}} \tilde{\lambda}_m(\tilde{\mu}_m) m^{2k/d} < \infty, \qquad k = 1, 2 \tag{3.20}$$

with $\tilde{\mu}$ *as in* (3.2a). *Then the solution* (Φ, μ) *satisfies* $\Phi \in X_\Lambda^k$ [*cf. Definitions* (2.2)–(2.3)] *and the same is true for any solution of the SP eigenmatrix problem* (2.6) *which is derived from* Φ *by a unitary transformation of the type* (2.7b).

Remarks. Property (3.20) holds for the Fermi function for all $k \in \mathbb{N}$; this gives higher-order regularity of the eigensolution Φ if the data $\tilde{V}$ and n_0 are sufficiently regular.

Theorem 3.5 is true also for $d \geq 4$ under certain smallness assumptions on the data (e.g., the period L or n_D or $\tilde{V}$).

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